Hydrogen influence on plastic relaxation at grain boundaries in aluminum

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The paper presents a molecular dynamics (MD) study of the effect of H atoms on the mechanisms of plastic deformation of Al systems during shear deformation with different structures and specific energies of grain boundaries (GB). MD calculations are performed using the LAMMPS package [1]. To describe interatomic interactions for the Al-Cu system the potential [2] is used, for the Al-H system from [3], the interaction of Cu-H was described using the Lennard Jones potential. The study carried out for the systems containing H atoms on the GB in the concentration of 1-10 at.% showed that the presence of H atoms on the GB for most of the systems did not change the mechanism of plastic relaxation. For almost all the systems considered, H strengthening was observed due to the fixation of the boundary by H atoms and an increase in stresses in the system. For a system with a misorientation angle of 36.87° and a specific GB energy of 694 mJ/m^2, with the addition of H atoms, an increase in stress to 715 MPa is observed; for this system without H, the maximum stress is 525 MPa. Softening with the addition of H atoms was observed for the 36.87° system and the specific energy of the GB of 467 mJ/m^2, the shear stresses decreased from 1020 MPa for the system without H to 894 MPa for the system with 10% concentration of H atoms near GB.

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